

FIG. 1

APPENDIX
 CLASS
 SUBCLASS
 ORAFIC

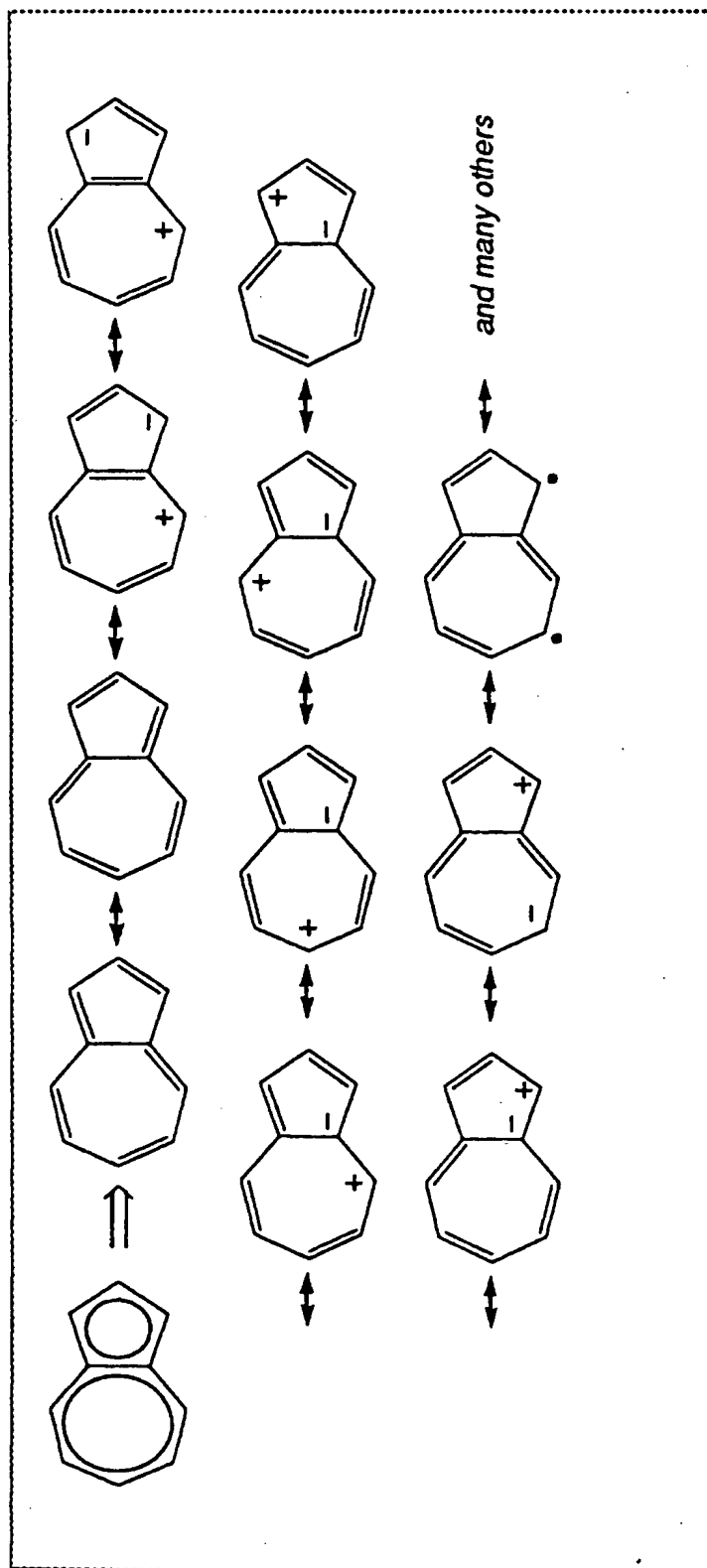


FIG. 2

3/37

APPARATUS	FIG.
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DRAWING	

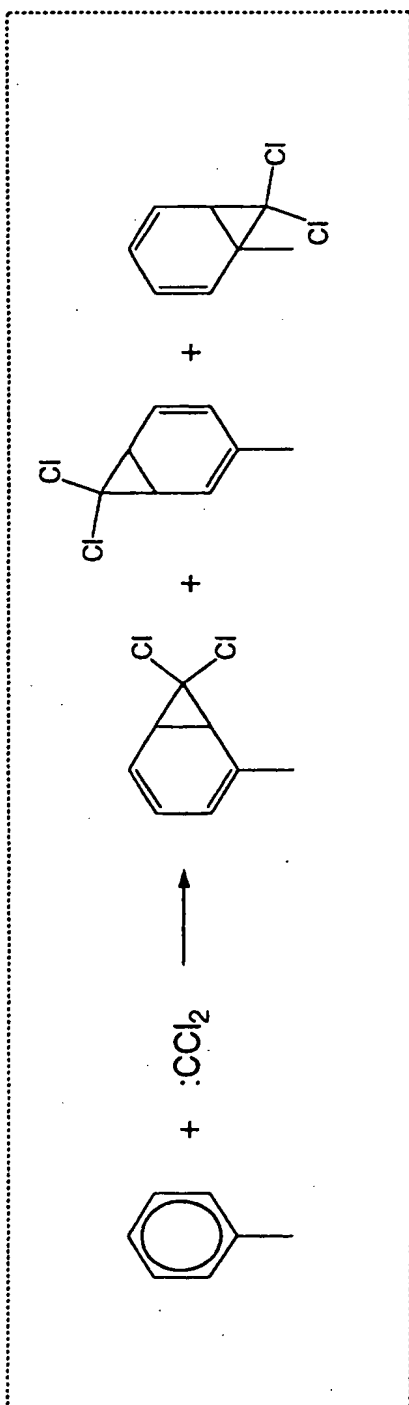


FIG. 3

FIG. 1	FIG. 2
FIG. 3	FIG. 4
FIG. 5	FIG. 6
FIG. 7	FIG. 8
FIG. 9	FIG. 10
FIG. 11	FIG. 12
FIG. 13	FIG. 14
FIG. 15	FIG. 16
FIG. 17	FIG. 18
FIG. 19	FIG. 20
FIG. 21	FIG. 22
FIG. 23	FIG. 24
FIG. 25	FIG. 26
FIG. 27	FIG. 28
FIG. 29	FIG. 30
FIG. 31	FIG. 32
FIG. 33	FIG. 34
FIG. 35	FIG. 36
FIG. 37	FIG. 38
FIG. 39	FIG. 40
FIG. 41	FIG. 42
FIG. 43	FIG. 44
FIG. 45	FIG. 46
FIG. 47	FIG. 48
FIG. 49	FIG. 50
FIG. 51	FIG. 52
FIG. 53	FIG. 54
FIG. 55	FIG. 56
FIG. 57	FIG. 58
FIG. 59	FIG. 60
FIG. 61	FIG. 62
FIG. 63	FIG. 64
FIG. 65	FIG. 66
FIG. 67	FIG. 68
FIG. 69	FIG. 70
FIG. 71	FIG. 72
FIG. 73	FIG. 74
FIG. 75	FIG. 76
FIG. 77	FIG. 78
FIG. 79	FIG. 80
FIG. 81	FIG. 82
FIG. 83	FIG. 84
FIG. 85	FIG. 86
FIG. 87	FIG. 88
FIG. 89	FIG. 90
FIG. 91	FIG. 92
FIG. 93	FIG. 94
FIG. 95	FIG. 96
FIG. 97	FIG. 98
FIG. 99	FIG. 100

4/37

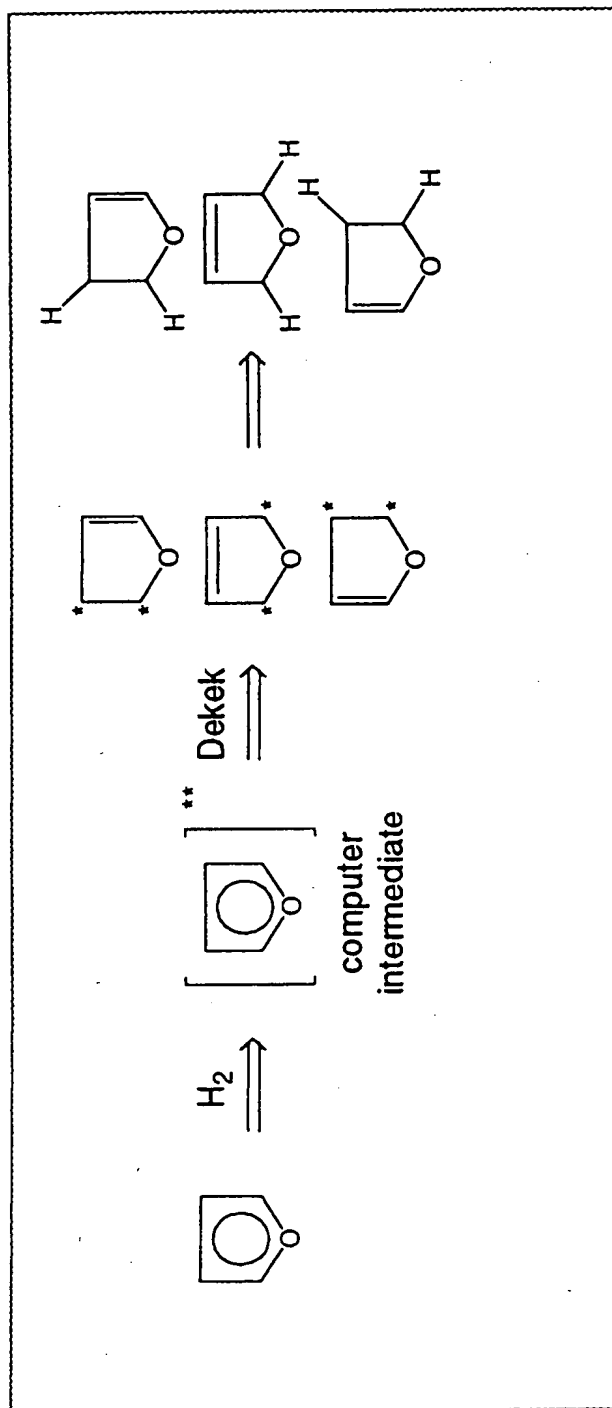


FIG. 4

5/37

ANALYST	FIG.
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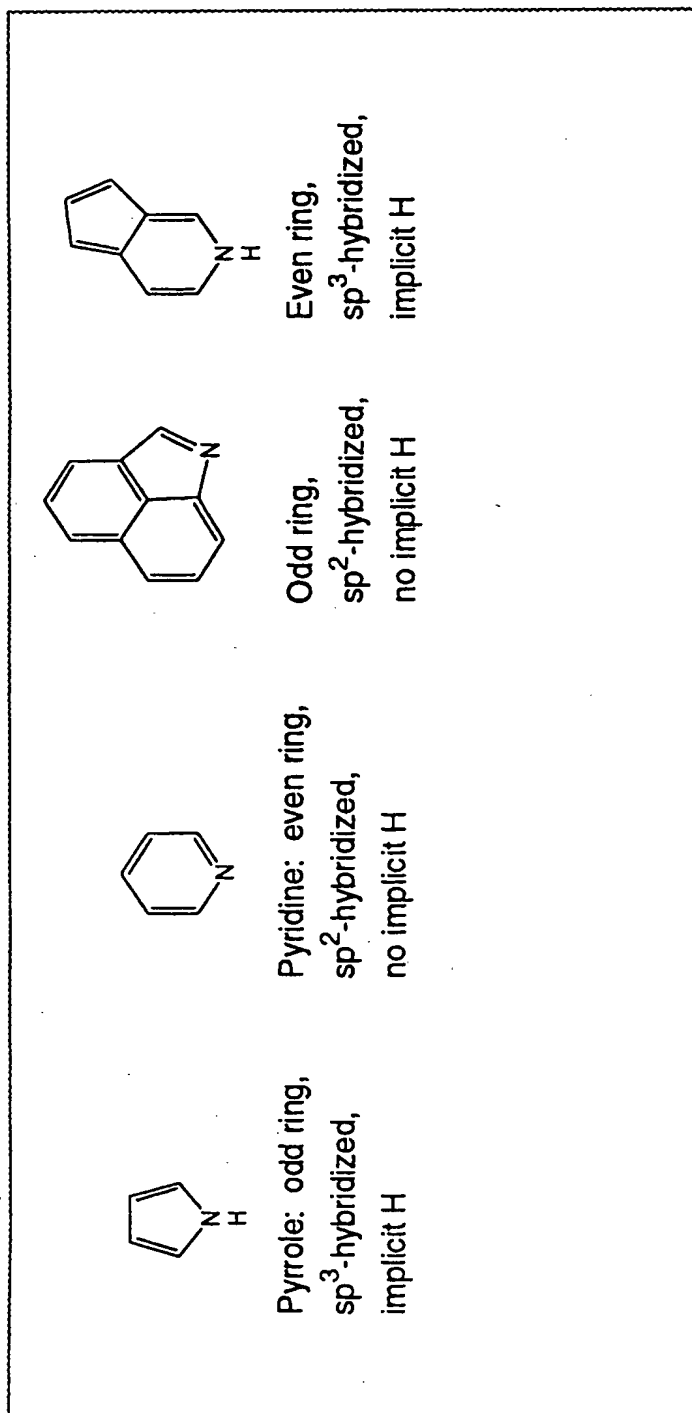


FIG. 5

APPROVED	FIG.
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6/37

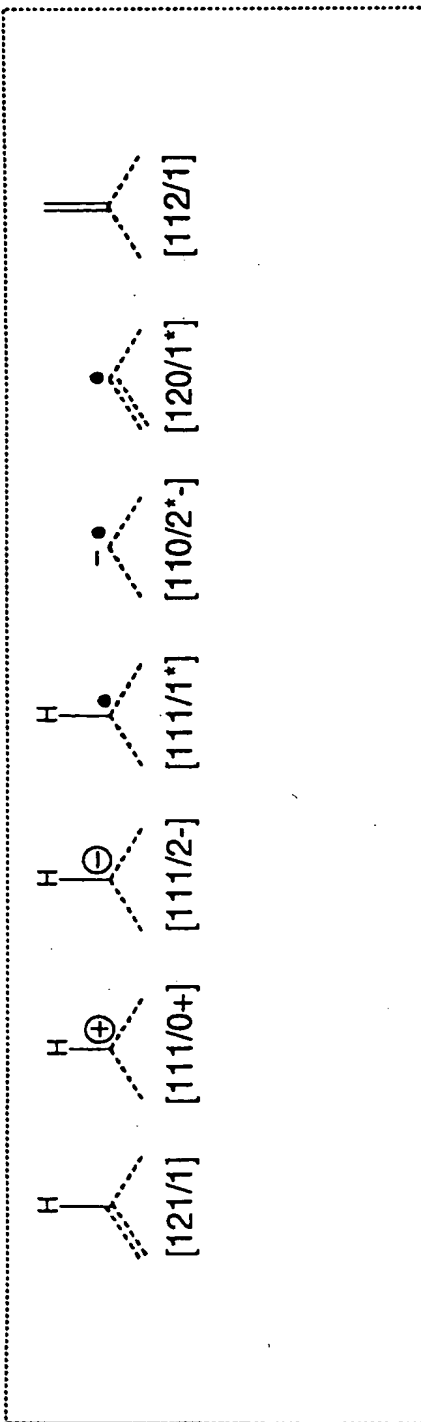


FIG. 6

7/37

Table 1. Selected Electronic State/Valence Distributions^a

<u>Elm</u>	<u>Chrg</u>	<u>Rad</u>	<u>Bd#1</u>	<u>Bd#2</u>	<u>#Extern Bds^b</u>	<u>#e's Contrib</u>	<u>Shorthand</u>	<u>Structure</u>
B			1	2	0	1	[120/1]	B-1
B			1	1	1	0	[111/0]	B-2
B	-1		1	2	1	1	[121/1-]	B-3
C			1	2	1	1	[121/1]	C-1
C	+1		1	1	1	0	[111/0+]	C-2
C	-1		1	1	1	2	[111/2-]	C-3
C		•	1	1	1	1	[111/1*]	C-4
C			1	1	2	1	[112/1]	C-5
N			1	2	0	1	[120/1]	N-1
N			1	1	1	2	[111/2]	N-2
N	+1		1	2	1	1	[121/1+]	N-3
N	+1	•	1	1	1	1	[111/1+*]	N-4
O			1	1	0	2	[110/2]	O-1
O	+1		1	1	1	2	[111/2+]	O-2
O	+1		1	2	0	1	[120/1+]	O-3
P like N ^c								
P			1	2	2	1	[122/1]	P-1
S like O								
S			2	2	0	2	[220/2]	S-1
Cl	+1		1	1	0	2	[110/2+]	Cl-1
Cl			1	2	2	1	[122/1]	Cl-2
Cl			1	2	4	1	[124/1]	Cl-3

FIG. 7

8/37

APPR. FIG.
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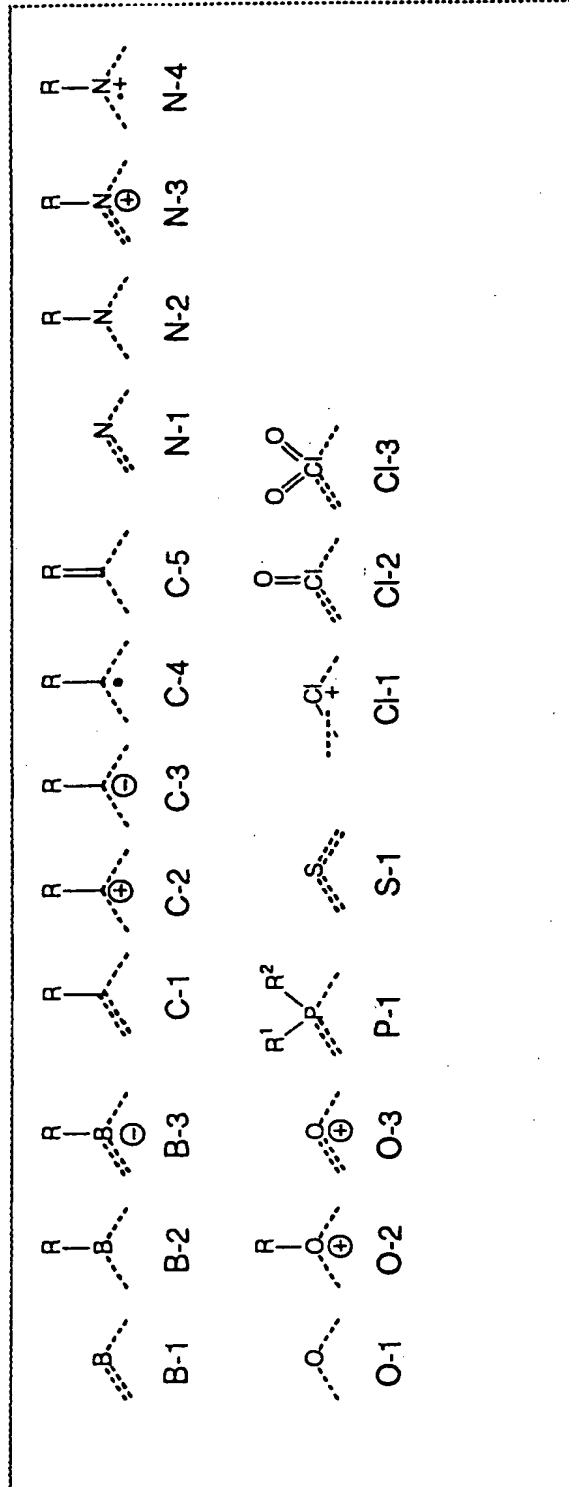


FIG. 8

ACTING	1.1.1.1.
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9/37



Table 2. Procedure Control Flags

Flag	Meaning
kDontAssumeImpH	Otherwise, heteroatoms might carry undrawn hydrogens.
kIfFailWithOneSystem_FailWithAll	If given two or more delocalized systems and one fails, the molecule is returned unchanged, and the procedure fails.
kDoNotCreateCharges	Do not create zwitterions, i.e., more charges than necessary to achieve the system's net charge.
kDoNotCreateRadicals	Do not create more than one radical.
kConfineChargesToHeteroatoms	All charged atoms must be heteroatoms.
kConfineRadicalsToHeteroatoms	All atoms with an unpaired electron must be heteroatoms.
kFavorMultiplyBondedHetero	When a system can support more or fewer multiple bonds, favor the form with more multiple bonds (even if it is anti-aromatic).
kDisfavorAntiaromaticSystems	Use this flag in conjunction with the previous.
kSolutionMustBeFullyAlternating	Bonds must alternate as single and double.

FIG. 9

Diagram illustrating the iterative process of finding a solution for the 3D isomorphism problem, showing the evolution of a graph structure from an initial state to a final state.

The process starts with an initial graph (1) and proceeds through several iterations (2) through (7), each showing a graph structure and its associated label (1) through (7).

The graphs are labeled (1) through (7) and are connected by arrows indicating the sequence of transformations.

The final state (7) is labeled "success", indicating that a solution has been found.

The process is labeled "failure" at the top, indicating that the initial attempt to find a solution failed.

FIG. 10

Table 3. Meanings of bits in the ESVD Screening Bitmask (ESB) and Atom Screening Bitmask (ASB)

<u>Bit #</u>	<u>Description</u>	<u>Bit #</u>	<u>Description</u>
0	Has an internal single bond	8	Charge = 0
1	Has two internal single bonds	9	Charge = +1
2	Has an internal double bond	10	Charge = -1
3	Has two internal double bonds	11	Charge ≠ -1
4	Has an external bond	12	Charge ≠ +1
5	Does <i>not</i> have an external bond	13	Radical present
		14	Radical not present

FIG. 11

FIG. 12	
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12/37

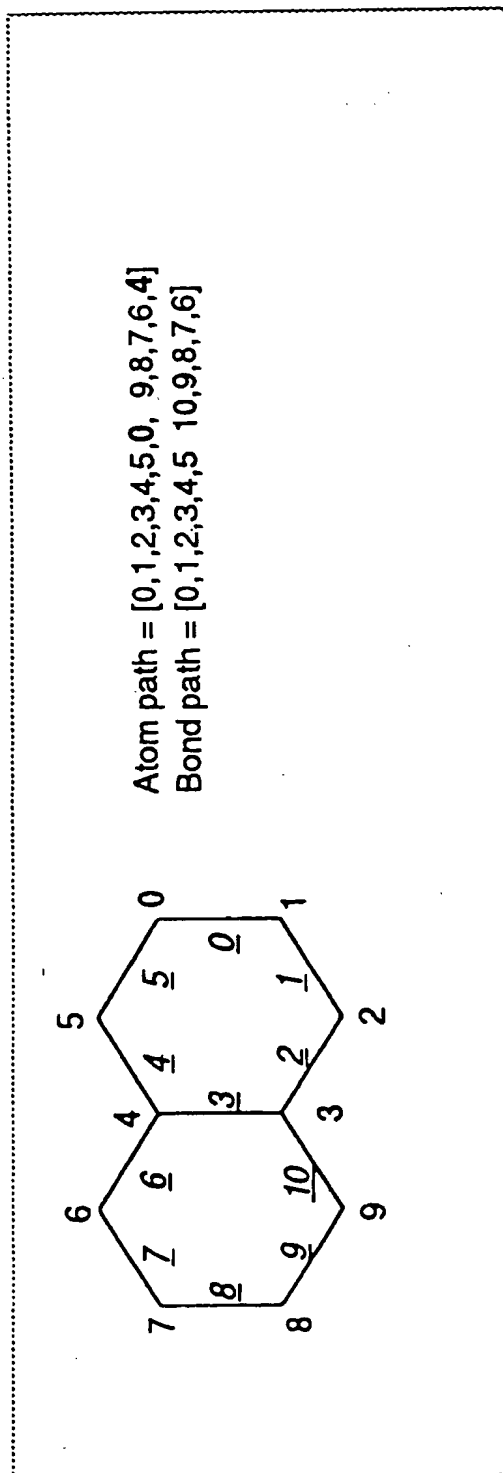


FIG. 12

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13/37



<u>Action #</u>	<u>Action</u>	<u>Atom / Bond</u>	<u>Action #</u>	<u>Action</u>	<u>Atom or Bond</u>
1	Assign ESVD	Atom 0	14	Assign Bond	Bond 10
2	Assign Bond	Bond 0	15	Assign ESVD	Atom 9
3	Assign ESVD	Atom 1	16	Assign Bond	Bond 9
4	Assign Bond	Bond 1	17	Assign ESVD	Atom 8
5	Assign ESVD	Atom 2	18	Assign Bond	Bond 8
6	Assign Bond	Bond 2	19	Assign ESVD	Atom 7
7	Assign ESVD	Atom 3	20	Assign Bond	Bond 7
8	Assign Bond	Bond 3	21	Assign ESVD	Atom 6
9	Assign ESVD	Atom 4	22	Assign Bond	Bond 6
10	Assign Bond	Bond 4	23	Verify completed	Atom 4
11	Assign ESVD	Atom 5	24	Complete	---
12	Assign Bond	Bond 5			
13	Verify completed	Atom 0			

FIG. 13



Table 4. The Actions Comprising a Strategy

<u>Action</u>	<u>Applies To</u>	<u>Explanation</u>
Assign ESVD	Atom	Find the ESVD's for the current atom that are compatible with its environment. The best one is used directly, and if there is more than one, the rest are queued.
Assign Bond	Bond	Assign a bond order to the current bond, consistent with the ESVD of the previous atom, i.e. the (earliest occurring) atom adjacent to the bond. (The bond's other atom has not been encountered yet, unless the bond closes a ring. Even in this case, the other atom's environment is not taken into account. It will be checked in the next Action.)
Verify Completed	Atom	This Action is taken just after the last bond in a ring or acyclic chain is fixed. Ordinarily the bonds of an atom are sure to be compatible with its assigned ESVD because its ESVD was picked to be compatible with the bond leading to it, and the bond leading away from it was selected to be compatible with its ESVD. However, a ring closure atom has not had its ESVD checked with respect to the ring closure bond, nor has a terminal atom in an acyclic chain. Thus, in this Action the atom is checked to verify that its final bonding environment is compatible with its ESVD.
Complete	---	Signifies that the path is completed, and all atoms have been assigned compatible ESVD's and bond orders. If the net charge or radical count of the putative solution is wrong, the solution is rejected. If the solution is perfect, as defined elsewhere, it is returned directly and the procedure terminates. Otherwise, if it is the best solution yet, it displaces the previous best candidate.

FIG. 14
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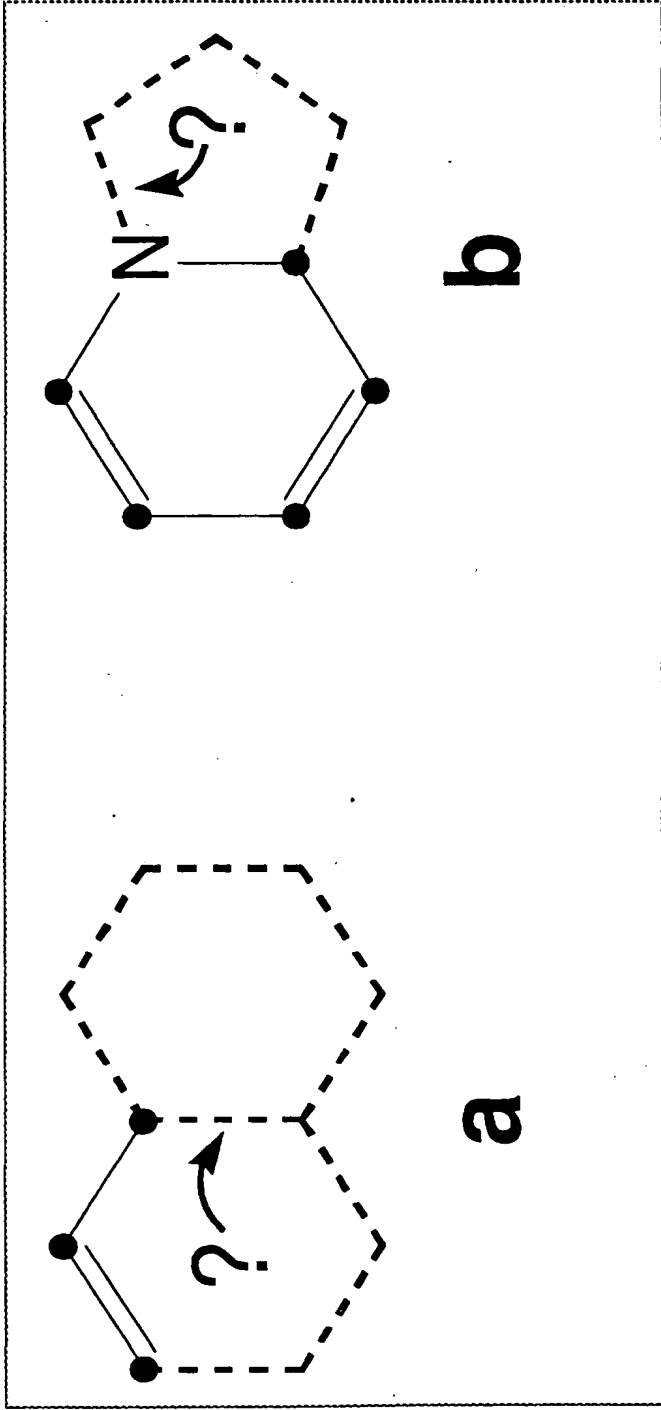


FIG. 15

FIG. 15	
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17/37

FIG.
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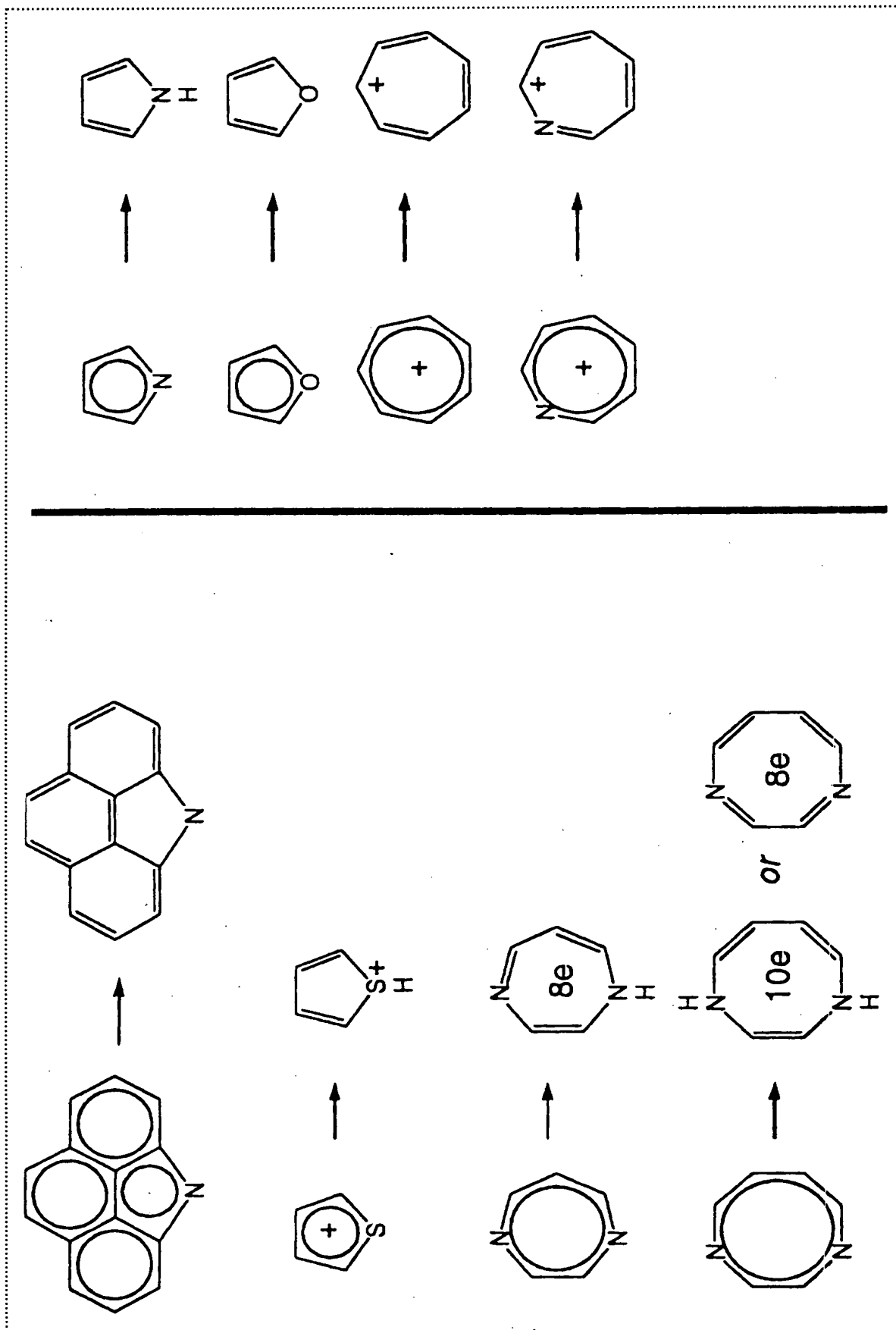


FIG. 17

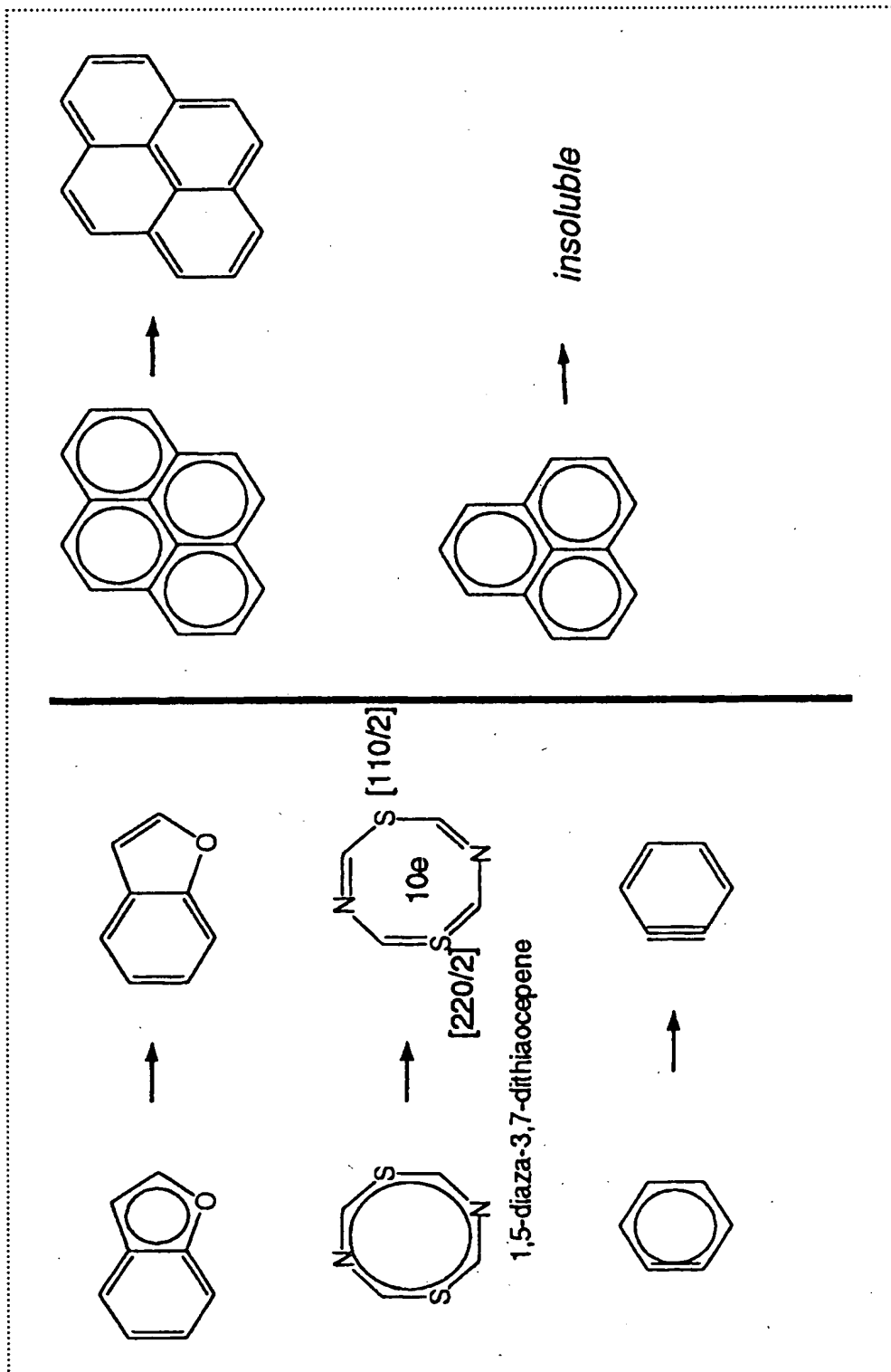


FIG. 18

APPENDIX	FIG.
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19/37

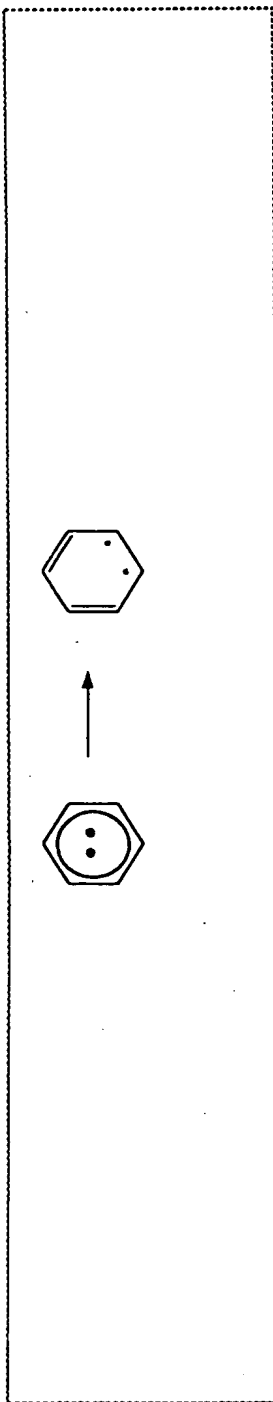


FIG. 19

20/37

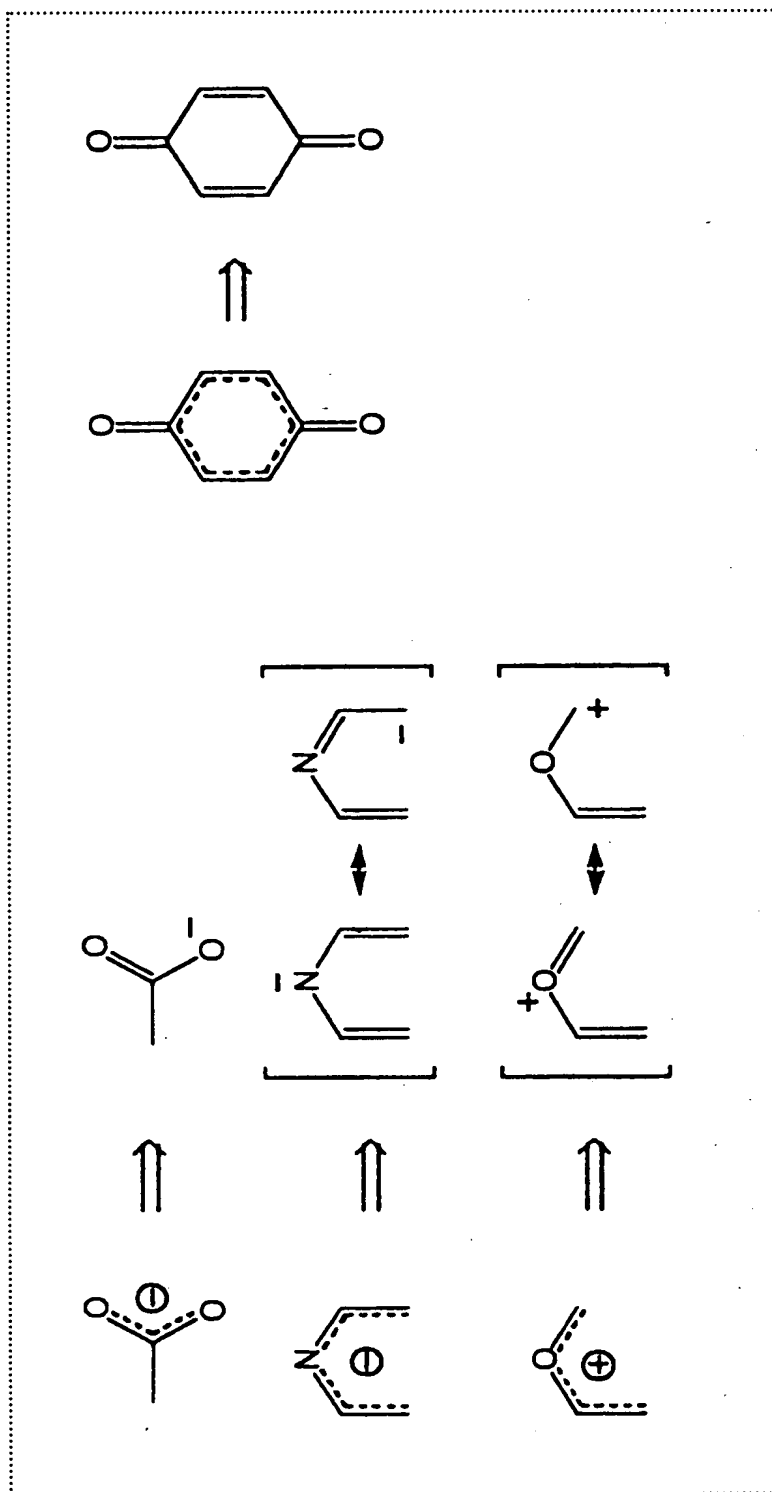


FIG. 20

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 DRAFTS: [Signature]
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21/37

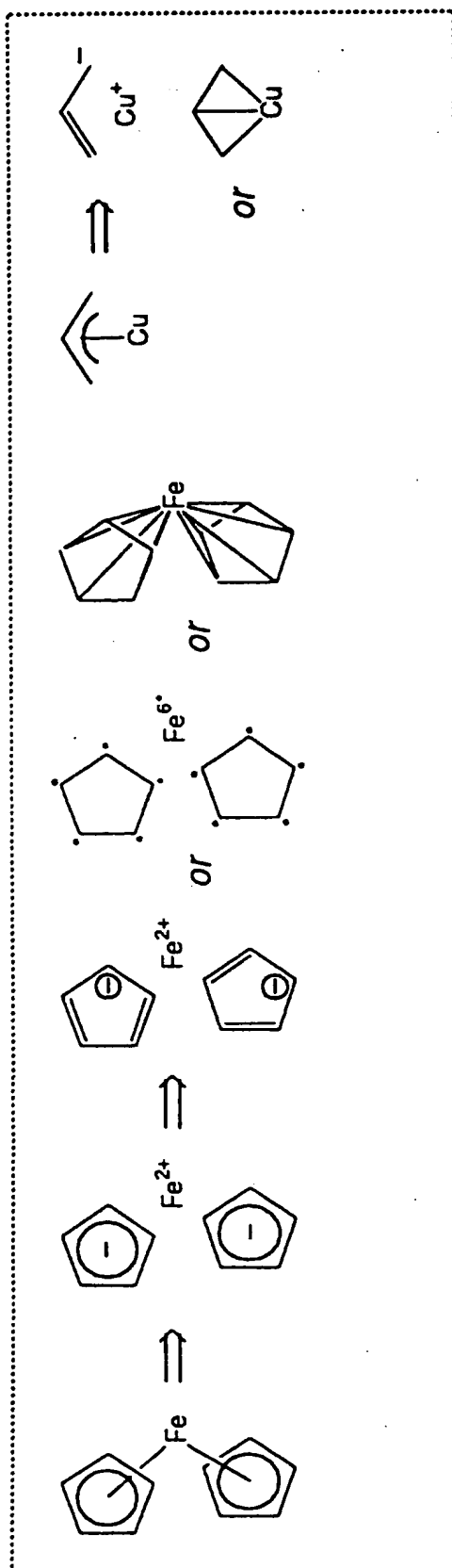


FIG. 21

22/37

FIG.
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1000

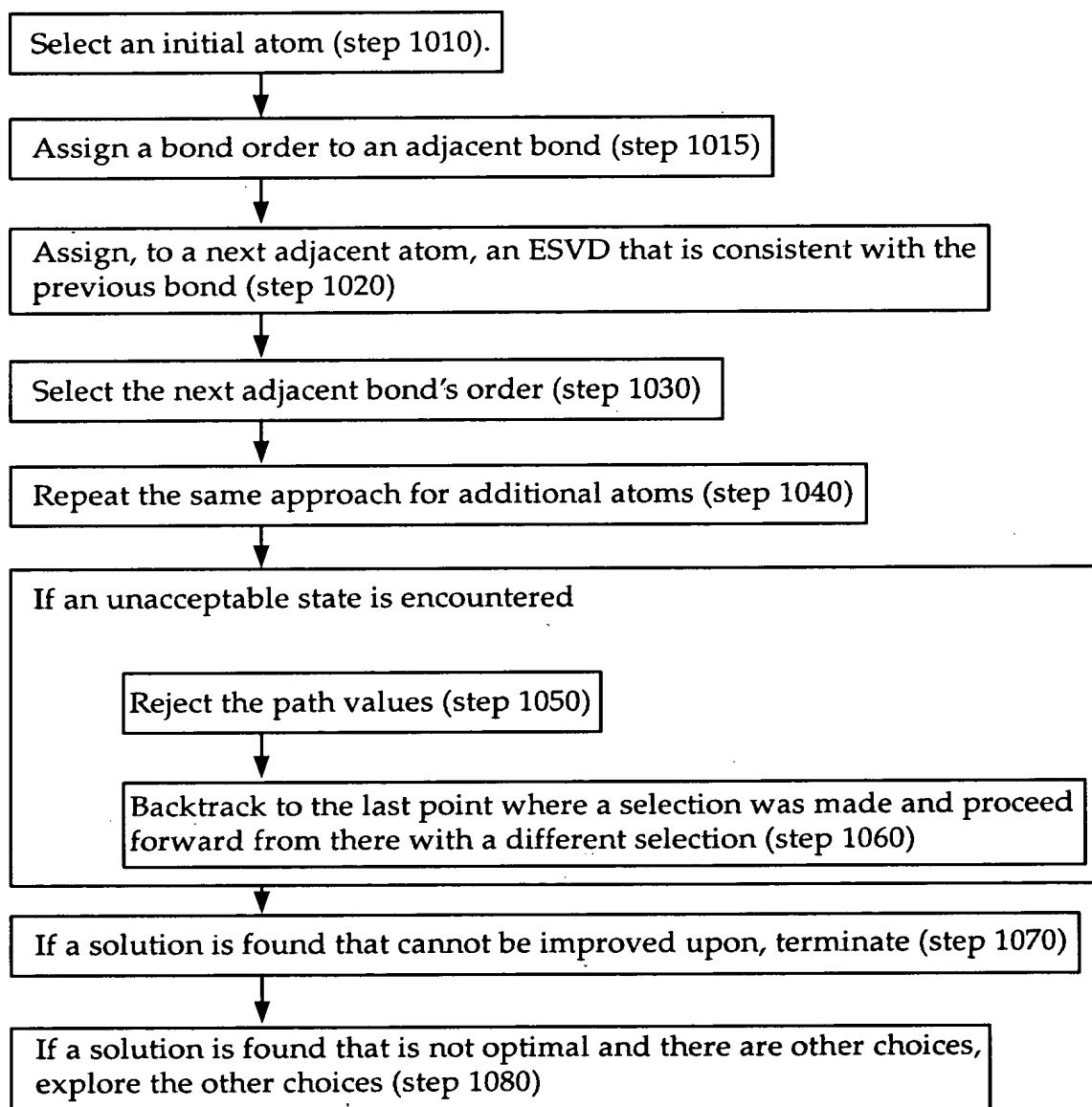


FIG. 22

23/37

2000

FIG. 23A
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Identify discrete (i.e., not adjacent) delocalized systems present in the structure (step 2010).

Select any delocalized bond that has not already been treated (step 2020)

Add all adjacent delocalized bonds (step 2030)

Continue to add delocalized bonds adjacent to those just found, until no new bonds are added (step 2040)

For each of the identified delocalized systems (step 2050)

Analyze *DS* for characteristics (step 2060)

Note the total charge and radical count required of the pi system (step 2070)

Calculate the internal coordination number ("ICN") of each atom (step 2080)

Identify bonds in *DS* that must be fixed, as a consequence of having an adjacent fixed multiple bond (step 2090)

Develop a path through *DS* (step 2100)

Construct the strategy list (step 2110)

Identify ring systems (step 2120)

Set the best solution ("BS") to "undefined" (step 2130)

E

FIG. 23A

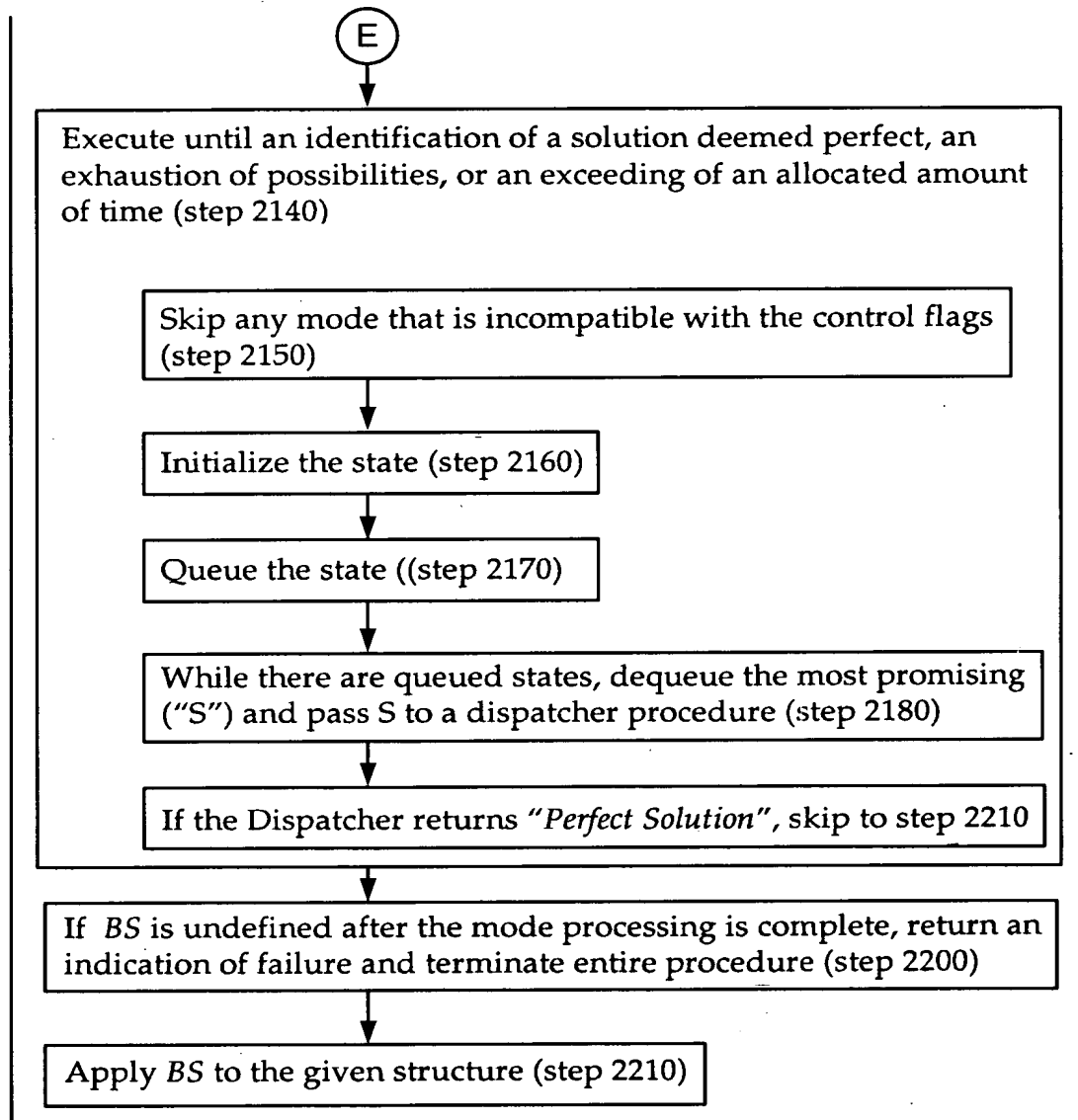


FIG. 23B

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3000

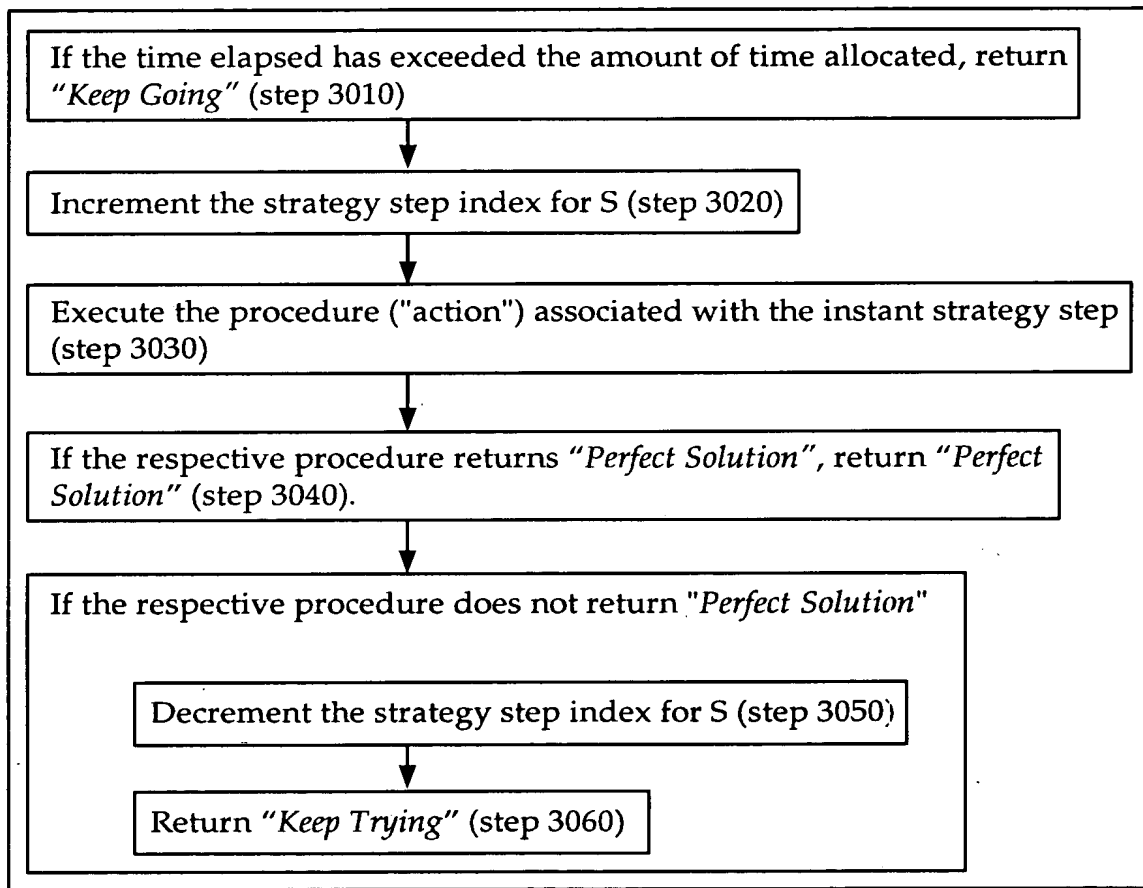


FIG. 24

26/37

4000

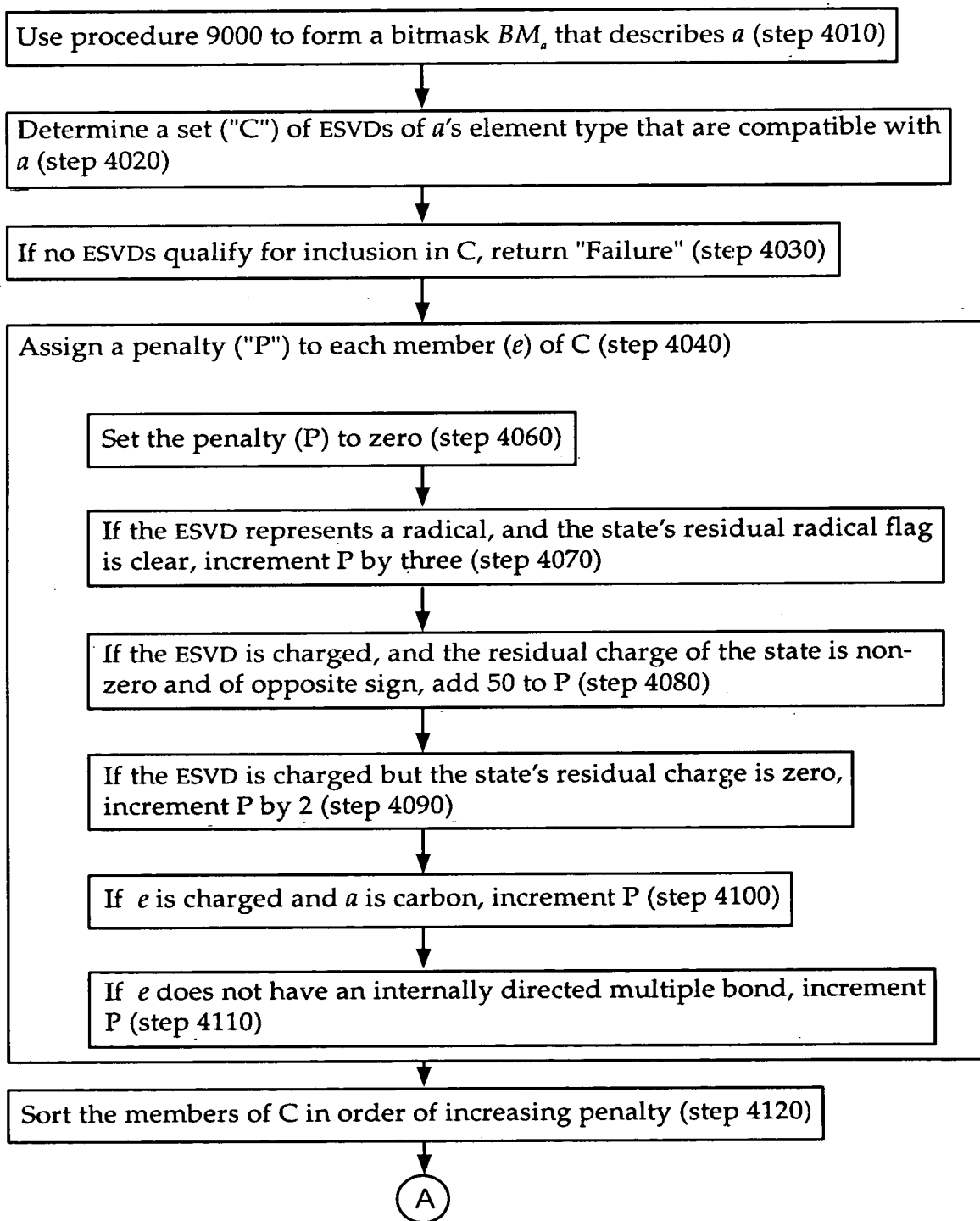


FIG. 25A

27/37

(A)

Queue inferior ESVDs for later consideration (step 4130)

For each member (C_i) of C except the first (i.e., the best), execute the following steps 4150 - 4180 (step 4140)

Copy the current state is copied to a new state, q (step 4150)

Set the ESVD of atom a in q to C_i (step 4160)

Increment the strategy step counter for q (step 4170)

Insert q into the priority queue (step 4180)

Apply the best ESVD to S (step 4190)

Update the state variables having to do with atomic properties (step 4210)

Subtract the ESVD's charge from the state's residual charge (step 4220)

If the ESVD has an unpaired electron, toggle the state's residual radical flag (step 4230)

Invoke the Dispatcher recursively (step 4240)

If the Dispatcher returns "Perfect Solution", return the same and terminate (step 4250)

Restore S to its value before the best ESVD was applied (step 4260)

(B)

FIG. 25B

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28/37

FIG.	CLASS
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Return "Keep Trying" (step 4270)

FIG. 25C

29/37

5000

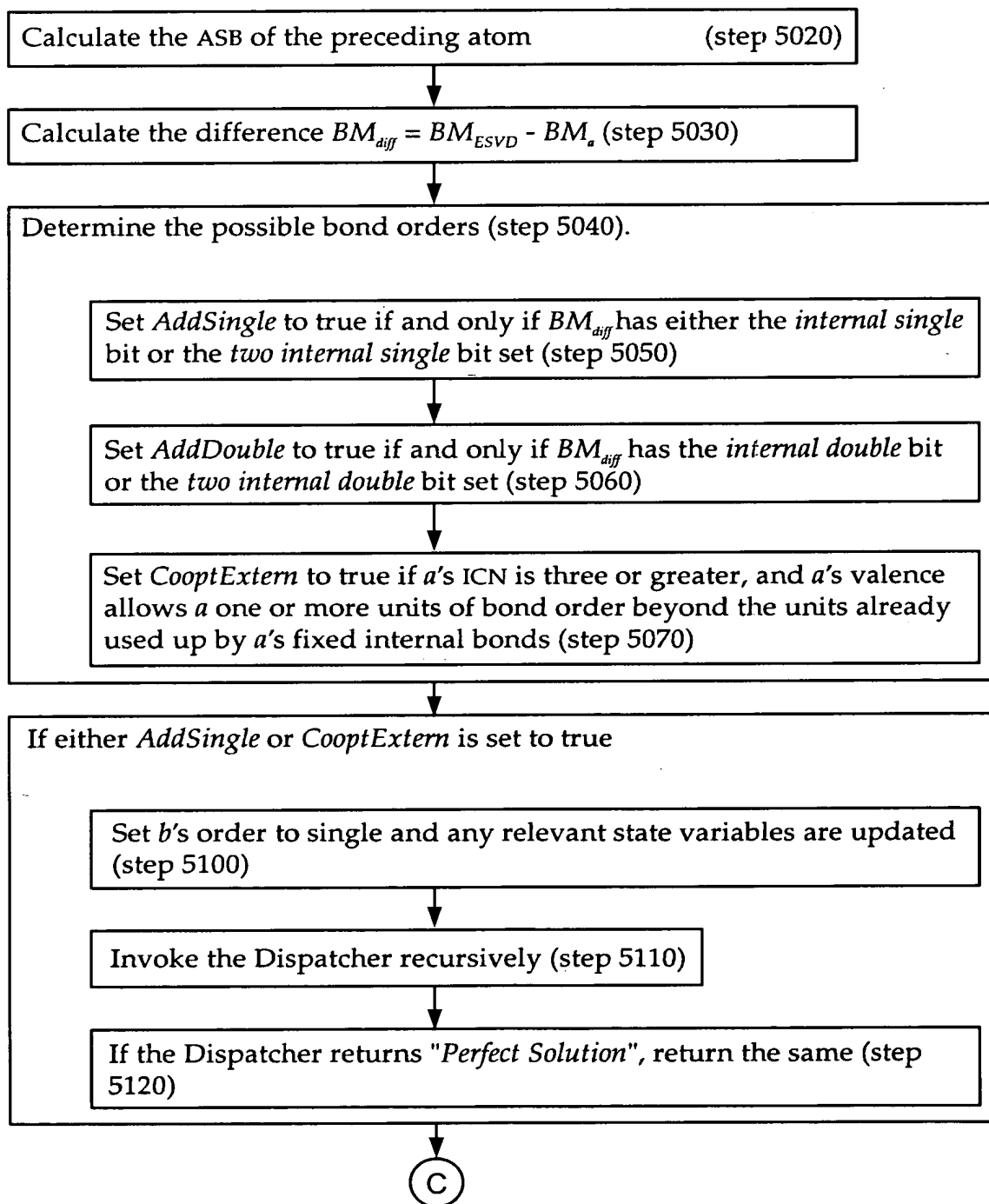


FIG. 26A

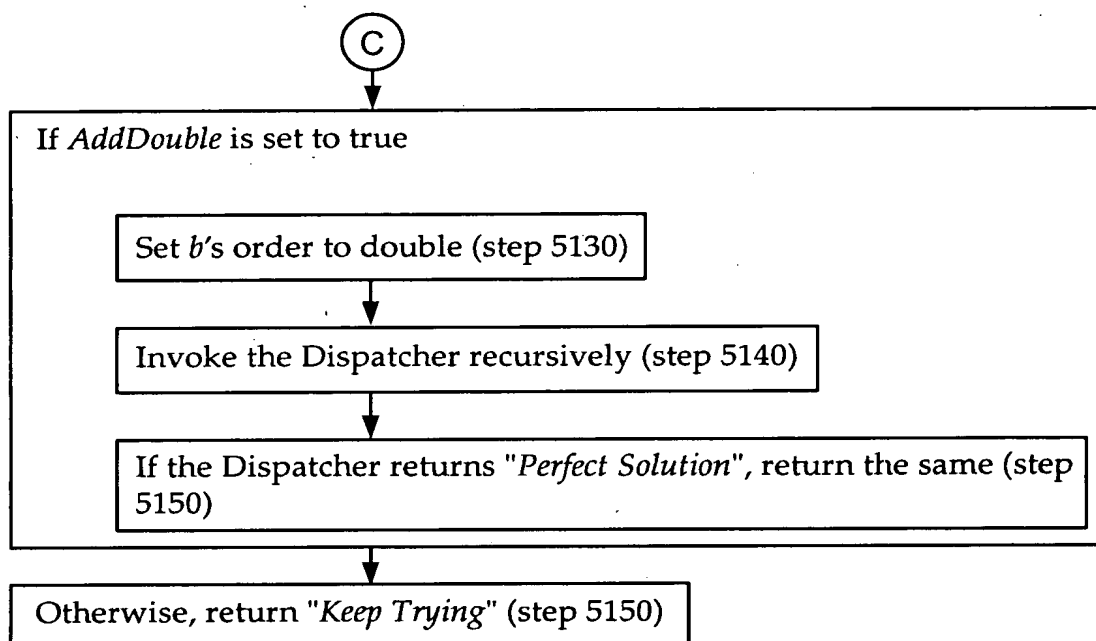


FIG. 26B

FIG. 27
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6000

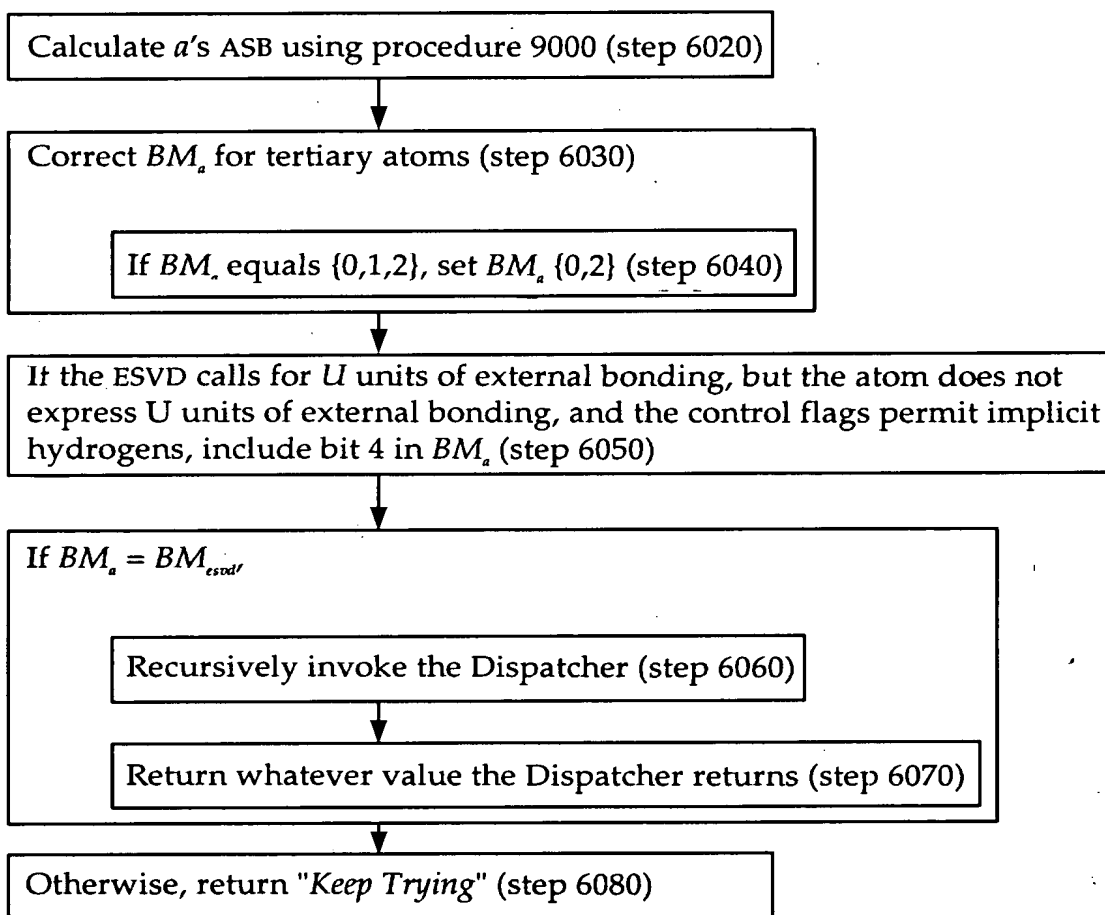


FIG. 27

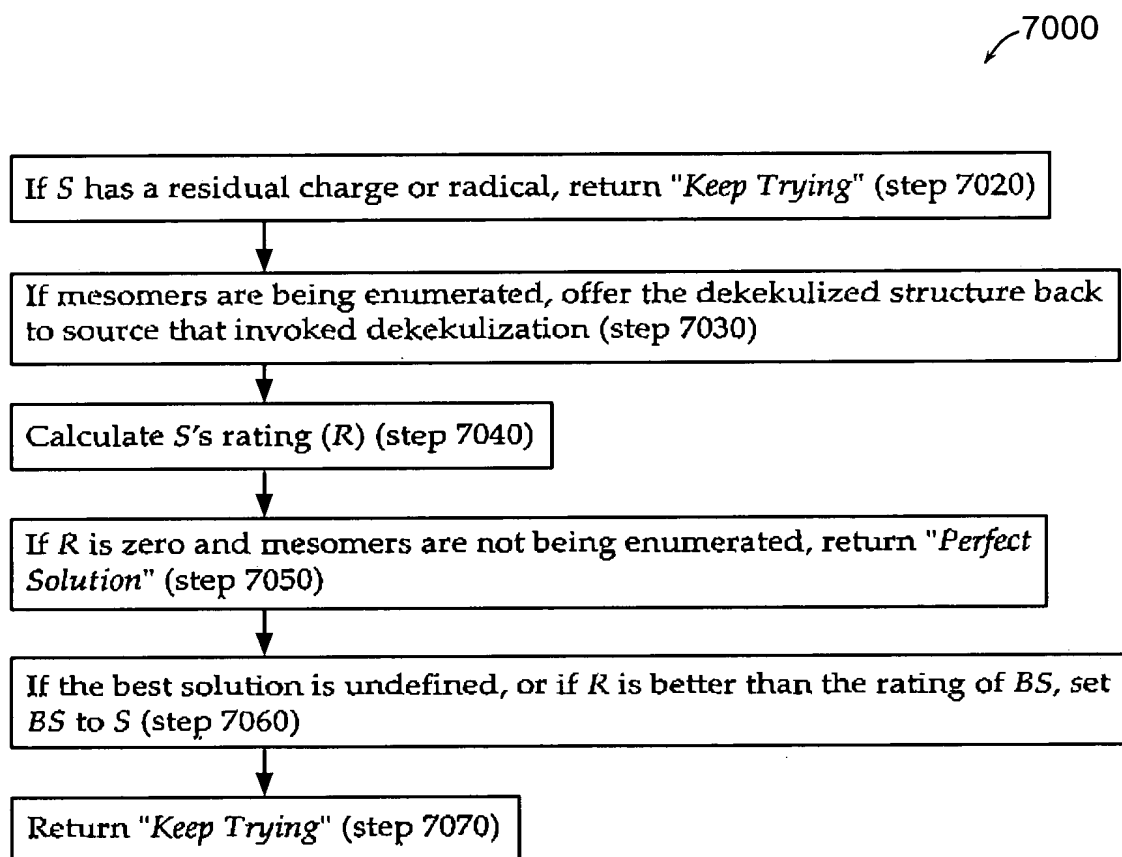


FIG. 28

8000

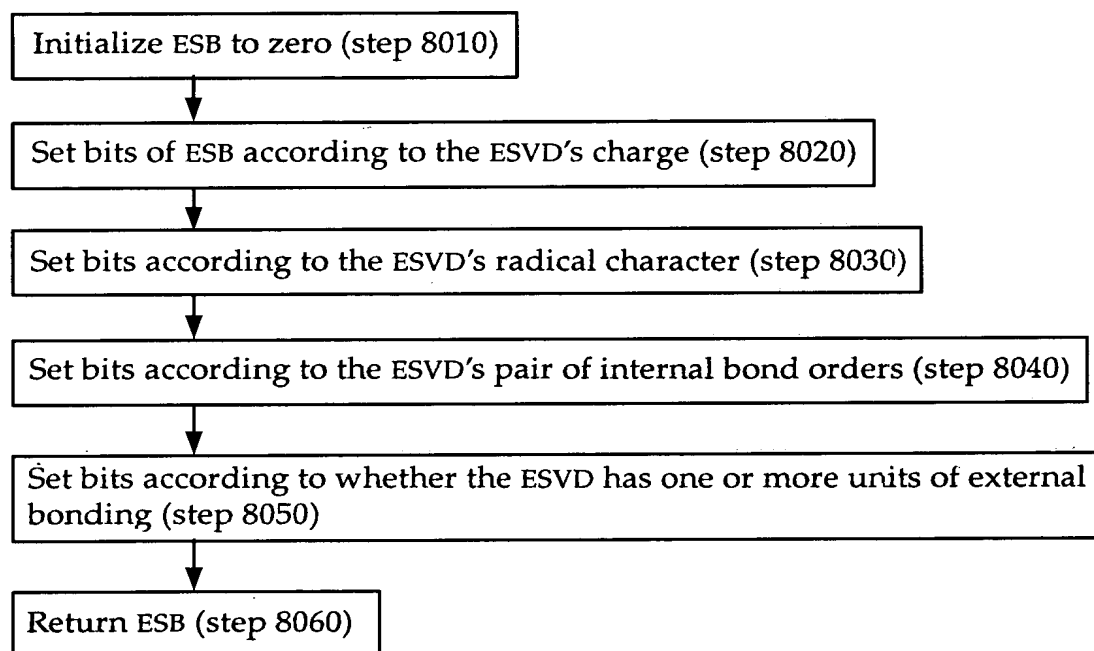


FIG. 29

9000

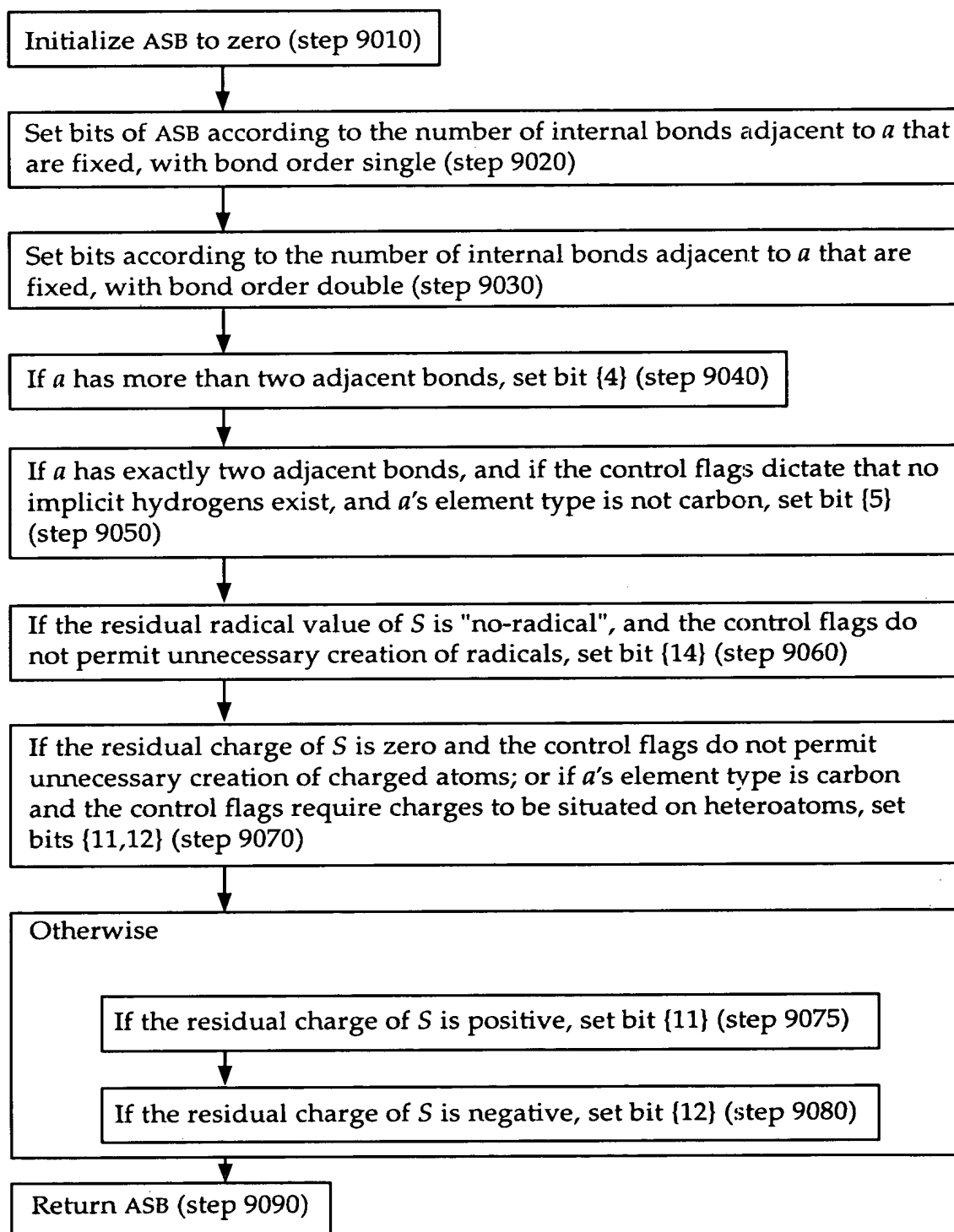


FIG. 30

35/37

10000

FIG.
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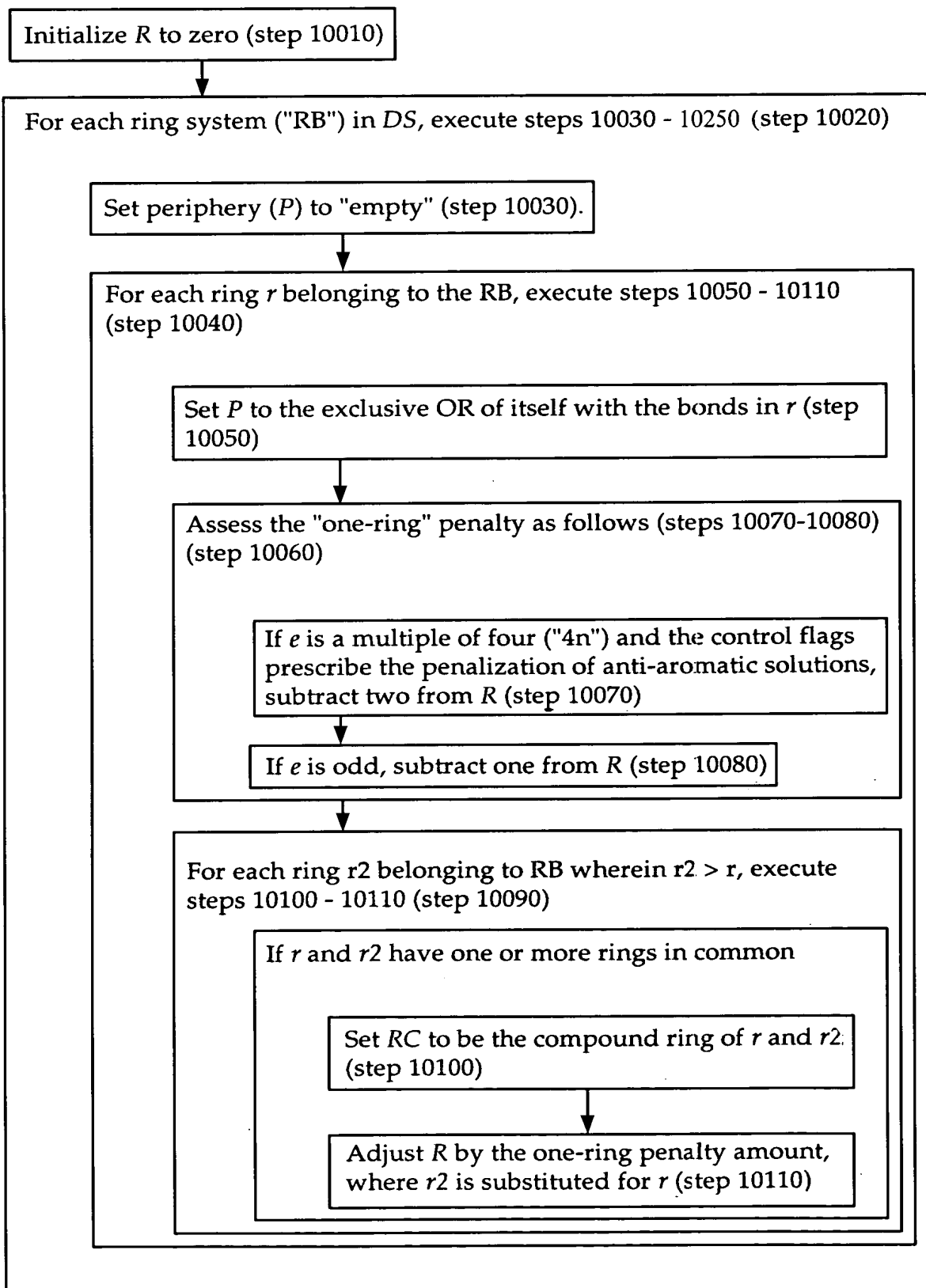


FIG. 31A

36/37

If there are three or more rings in RB

Take $r3$ to be the compound ring represented by P
(step 10120)

Adjust R by the one-ring penalty amount, where $r3$ is
substituted for r (step 10130)

Apply a significant penalty for gratuitous charges and radicals
(steps 10160 - 10180) (step 10140)

Take NSC to be the number of superfluous charges (step
10160)

Take NSR to be the number of superfluous radicals (step
10170)

Reduce the score by ten times $(NSC + NSR)$ (step 10180)

Apply a small penalty for locating a charge on a carbon rather than
an available heteroatom (steps 10200 - 10220) (step 10190)

Take NCC to be the number of charged carbon atoms in S
(step 10200)

Take NNH to be the number of neutral heteroatoms in S
(step 10210)

If NCC exceeds NNH , reduce R by $(NCC - NNH)$ (step 10220)

Penalize pairs of adjacent atoms having identical, either empty or
full, orbitals (step 10230)

D

FIG. 31B

37/37

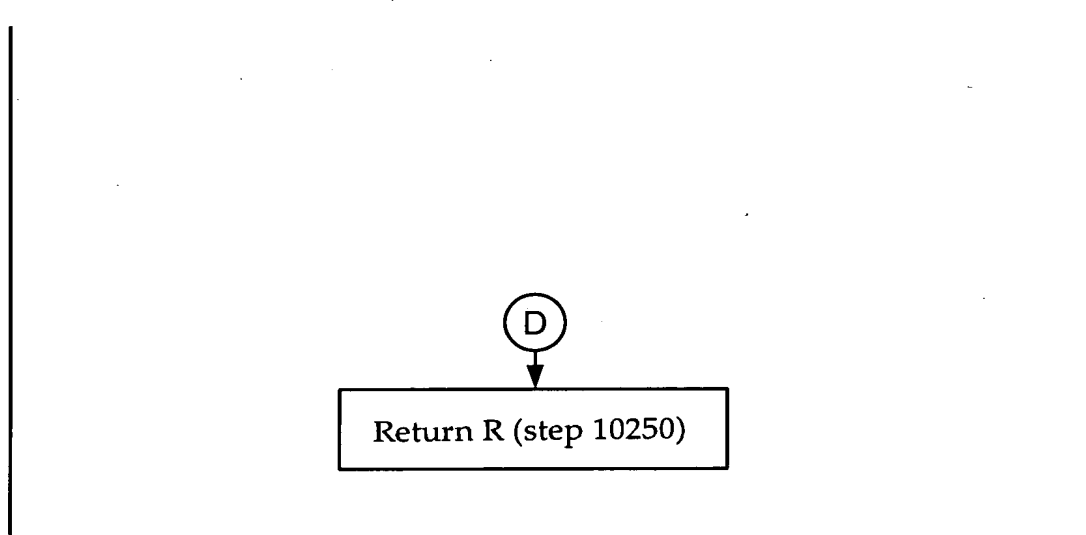


FIG. 31C

FIG. 31C
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